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Process Intensification of the production of Di-Methyl Carbonate (DMC) using a New Synthesis and Design Process Intensification Methodology

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Abstract

Process Intensification (PI) is a means by which processes, whether new or existing, can achieve a more efficient and sustainable chemical process through the improvement of, for example, energy efficiency and waste generation. PI can be defined as the improvement of a process at the phenomena level which ultimately has an impact at the higher levels of a process, that is the functional and unit operations (Unit-Ops) levels. More specifically PI is the enhancement of the involved phenomena through the integration of Unit-Ops, functions and phenomena. Except for reactive distillation and dividing wall columns, the implementation of PI still faces hurdles [1]. For achieving PI via a systematic approach different methodologies exist, of which two are mentioned here, the task-based means-ends analysis developed by Sirrola [2] and the Unit-Ops based synthesis and design method for achieving PI developed by Lutze et al. [1]. These methods, which work at the Unit-Ops level, are limited to PI equipment already in existence and are therefore able to generate new integrations/combinations of intensified existing equipment but may not generate new/innovative PI solutions.

The objective of this work is threefold: (1) the development of a new/innovative systematic PI synthesis and design methodology, which includes model based synthesis/design and experimental based validation; (2) the development of a phenomena based synthesis and design method (PBS) which in addition to the knowledge-based (KBS) and Unit-Ops based (UBS) methods (thereby extending further, the application range) is one of the methodologies within the new PI methodology; and (3) the application of the new PI methodology to a case study - the production of di-methyl carbonate (DMC).

The new PI methodology has the following characteristics: (a) flexible for a wide range of applications (b) finds innovative (new) and predictive (existing) solutions and (c) model and experimental based validation of intensified options. The new PI methodology follows a systematic decomposition approach starting with a base case as a reference point. In Step 1 a general problem definition is determined. In Step 2 system information is collected based on thermodynamic data and the type of chemical/process systems that are identified. Using this data, the process is analysed and in Step 3, it is possible to use one or two or all of the PI methods. The three synthesis and design methods considered are the KBS, the UBS and the PBS. The KBS and UBS methods use knowledge stored in a knowledge-based tool on implemented PI equipment used for overcoming certain limitations/bottlenecks (LB's), for example, the use of reactive distillation for overcoming unfavourable equilibrium in a reaction. The PBS methodology not only uses the knowledge of the existing methodologies at the Unit-Ops level but also operates at a lower level of aggregation (i.e phenomena level), where the apriori knowledge of existing Unit-Ops is needed to some degree but also where new Unit-Ops, in principle, can be designed. In Step 4 the feasible flowsheets obtained from Step 3 are validated/ verified either through a model or experimental based analysis. At the end of Step 4 the best PI process candidate and the other feasible options are used to update the systems information. It should be noted that the degree of complexity increase from the KBS to PBS while the possibility of obtaining/generating novel PI equipment decreases from PBS to KBS.

A preliminary version for a phenomena-based synthesis/design (PBS) methodology has been developed [3] and consists of a six step workflow: Problem and objective function definition→ Process analysis using thermodynamic insights→ Identification of

LB's of the process together with the desirable and accompanying phenomena to overcome these LB's→ Phenomena building blocks are connected to form simultaneous phenomena building blocks (SPBs) which are screened for the most feasible connections using for example connectivity rules. The SPB's are then connected to form operations which are then connected to form flowsheets just as atoms are combined to form molecules→ Flowsheets are first screened using for example logical constraints and performance metrics to obtain feasible PI options→ The feasible flowsheets from are optimized with respect to the objective function with the end result being the identification of the best intensified process candidate. The emerging flowsheets consists of either novel or existing PI equipment. Defined phenomena are for example mixing, two-phase mixing, phase transition and phase separation. This preliminary version is now extended and implemented within the general PI synthesis design methodology.

In this presentation the PI synthesis and design methodology with focus on the PBS workflow will be highlighted together with the details of its application to the production of DMC. DMC is an important bulk chemical used as a solvent and fuel additive. It will be shown that the PBS methodology systematically generates, besides other options, the current intensified option proposed by the co-authors who have followed the UBS path of the combined methodology and is as follows: a reactive distillation column→ membrane separation →distillation.

References:

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